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The objective of this grant was to enable and enhance research and educational capabilities pertaining to analysis and visualization of computer-based simulations of materials systems, through the acquisiton of computer equipment and associated software for processing, analysis, visualization and animation of molecular dynamics simulation.

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"Analysis and Visualization of Simulated Dynamics in Complex Materials Systems"

Prepared for the AFOSR

by

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The objective of this grant was to enable and enhance research and educational capabilities pertaining to analysis and visualization of computer-based simulations of materials systems, through the acquisition of computer equipment and associated software for processing, analysis, visualization and animation of molecular dynamics simulation.

The above objective had been fully achieved through acquisition of the following major hardware and software:

1. SGI ORIGIN 2000 (4 processors)
2. SGI Octane
3. Memory and disk supplements to (1) and (2)
4. Video graphics board (SGI) and S-video capable VCR (Panasonic)
5. Hardware JPEG compression board
6. DLT and zip drives
7. HP Scanner
8. Various visualization and animation software including: Adobe (Premier, Photoshop, Illustrator and Acrobat), and IBM Data Explorer.

All the above (and additional memory enhancements to existing NCD graphics workstations) have been purchased and installed, and are currently in a full operative state.

The above equipment is used in conjunction with molecular dynamics (MD) simulations of a broad scope of material systems of basic and technological interest, including: frictional processes, thin-film lubrication, junction formations, collisional shock phenomena, crystallographic and electronic structures of nanocrystallites and their assemblies, gas-phase and surface supported clusters, chemical reactions in condensed-phases and catalyzed by small

particles, organic/inorganic interfaces, quantum wires and dots, and coatings.

By their nature, MD simulations, where the equations of motion of a system comprised of a large number of interacting particles (tens of thousands, and up to a million in modern simulations) are integrated numerically yielding the phase-space trajectory of the system, generate massive amounts of data. This is the case for both classical MD simulations employing tested semi-empirical potentials, as well as for ab-initio MD simulations where the ionic motion is evaluated on first-principles concurrently calculated potential energy surfaces (using in our studies self-consistent density functional theory in conjunction with non-local pseudopotentials).

We have employed the equipment purchased through this grant for analysis of results pertaining to several of our projects, including classical and ab-initio quantum molecular dynamics simulations. In particular we note our recent studies of friction control in boundary lubricated junctions (work supported by the AFOSR). In these investigations we discovered a novel method for controlling friction, through small amplitude oscillations during sliding of the confirmed solid boundaries in the direction normal to the shear plane. These oscillations frustrate ordering processes in the thin-lubricant film with a consequent reduction in friction (see J. Gao, W. D. Luedtke, and U. Landman, J. Phys. Chem. B 102, 5033 (1998)).

The above simulations employ our recently developed grand-canonical MD method where the confinement is immersed in a surrounding liquid which is under constant external pressure. The acquired equipment enabled visualization of the flow, and of disordering and ordering processes in the system, which proved crucial to interpretation of the results and to the development of the new friction control method. Additionally, we have prepared an animation video which illustrates the method. This video, as well as one concerned with nano-

elastohydrodynamics in non-uniform junctions, has been used in a number of presentations, including invited talks at the March 1998 American Physical Society (Los Angeles) and the April 1998 meeting of the American Chemical Society (Dallas).

Currently, we extended the simulations to systems composed of up to 250,000 particles in order to investigate scaling behavior with the confinement's physical dimensions. These large-scale simulations are performed with a parallelized version of our simulation codes, making optimal use of the parallel processing capability of the acquired 4 cpu SGI ORIGIN 2000. Visual analysis of the dynamics in these large systems allows us to explore the nature of ordering/ disordering processes in sheared lubricated films which are key to understanding their rheology and to the systematic development of model lubricants.

Finally, we remark that research using the newly acquired equipment is performed mostly by senior research scientists, post-doctoral fellows and graduate students, which are thus trained in the use of modern analysis and visualization techniques.